



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:33 PM UTC

PDB ID : 1EPP / pdb_00001epp
Title : ENDOTHIA ASPARTIC PROTEINASE (ENDOTHIAPEPSIN) COM-
PLEXED WITH PD-130,693 (MAS PHE LYS+MTF STA MBA)
Authors : Wallace, B.A.; Cooper, J.B.; Blundell, T.L.
Deposited on : 1994-07-27
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

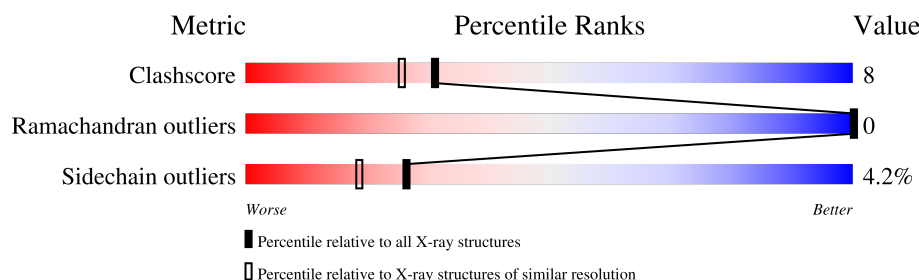
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	330	41% 52% 7%

2 Entry composition [i](#)

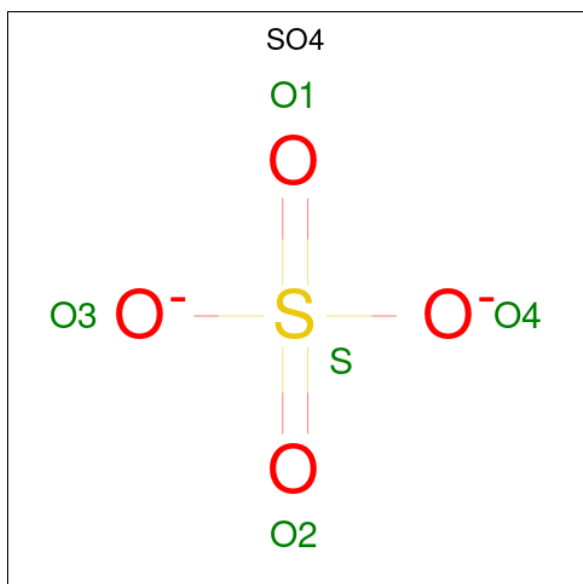
There are 4 unique types of molecules in this entry. The entry contains 2706 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ENDOTHAPEPSIN.

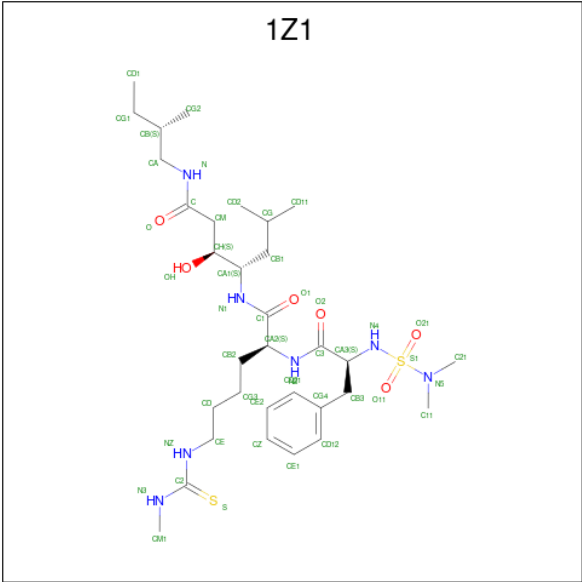
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	330	Total	C	N	O	S	0	0	0
			2389	1514	366	507	2			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is N-(dimethylsulfamoyl)-L-phenylalanyl-N-[(1S,2S)-2-hydroxy-4-[(2S)-2-methylbutyl]amino}-1-(2-methylpropyl)-4-oxobutyl]-N 6 -(methylcarbamothioyl)-L-lysineamide (CCD ID: 1Z1) (formula: C₃₂H₅₇N₇O₆S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	S	0	0
			47	32	7	6	2		

- Molecule 4 is water.

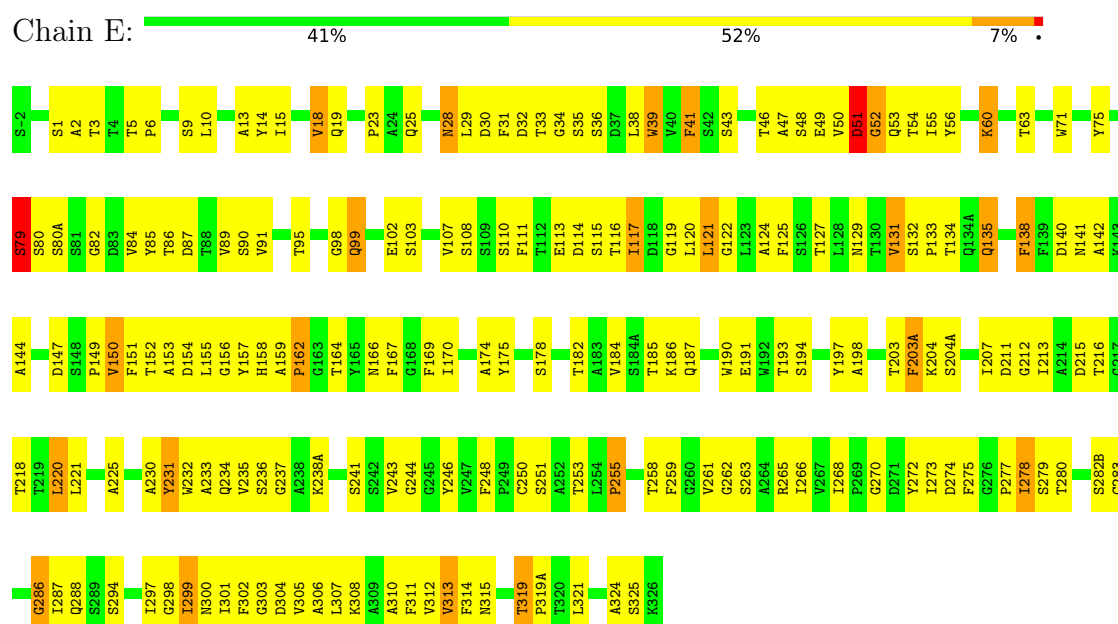
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	260	Total	O	0	0
			260	260		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: ENDOTHAPEPSIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.10 Å 75.60 Å 42.90 Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	84.0 (20.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.160 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2706	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 1Z1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	E	2.21	92/2445 (3.8%)	2.78	258/3345 (7.7%)

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	ASP	N-CA	13.11	1.54	1.46
1	E	39	TRP	N-CA	12.03	1.61	1.45
1	E	52	GLY	N-CA	9.23	1.58	1.45
1	E	278	ILE	CA-CB	-8.49	1.44	1.54
1	E	6	PRO	CA-CB	-8.15	1.42	1.53
1	E	51	ASP	CA-C	8.10	1.58	1.53
1	E	261	VAL	CA-C	7.96	1.62	1.52
1	E	41	PHE	N-CA	7.60	1.55	1.45
1	E	203(A)	PHE	CA-CB	-7.58	1.42	1.53
1	E	218	THR	CA-CB	-7.56	1.42	1.53
1	E	253	THR	N-CA	7.55	1.55	1.46
1	E	116	THR	C-N	-7.33	1.23	1.33
1	E	236	SER	N-CA	-7.21	1.37	1.46
1	E	53	GLN	CD-OE1	7.20	1.37	1.23
1	E	216	THR	CA-C	7.01	1.62	1.52
1	E	297	ILE	N-CA	6.96	1.54	1.46
1	E	80	SER	N-CA	6.92	1.54	1.46
1	E	149	PRO	C-O	-6.91	1.15	1.24
1	E	119	GLY	CA-C	6.72	1.59	1.52
1	E	187	GLN	CD-OE1	6.61	1.36	1.23
1	E	135	GLN	N-CA	6.59	1.53	1.46
1	E	157	TYR	N-CA	6.45	1.54	1.46
1	E	158	HIS	ND1-CE1	6.36	1.39	1.32
1	E	158	HIS	CD2-NE2	6.31	1.44	1.37
1	E	265	ARG	N-CA	6.29	1.53	1.46
1	E	85	TYR	CA-C	6.27	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	169	PHE	CA-CB	-6.24	1.43	1.53
1	E	19	GLN	CD-OE1	6.20	1.35	1.23
1	E	302	PHE	CA-C	-6.19	1.45	1.53
1	E	134	THR	N-CA	6.13	1.53	1.46
1	E	46	THR	N-CA	6.11	1.53	1.46
1	E	272	TYR	CA-C	6.10	1.61	1.52
1	E	193	THR	N-CA	-6.05	1.39	1.46
1	E	95	THR	CA-C	-6.05	1.45	1.52
1	E	38	LEU	CA-C	6.03	1.60	1.52
1	E	116	THR	C-O	5.97	1.31	1.24
1	E	32	ASP	CA-CB	5.92	1.62	1.53
1	E	237	GLY	N-CA	5.91	1.52	1.45
1	E	262	GLY	N-CA	5.91	1.54	1.45
1	E	13	ALA	CA-C	-5.89	1.45	1.52
1	E	131	VAL	CA-CB	-5.86	1.47	1.54
1	E	300	ASN	CG-OD1	5.83	1.34	1.23
1	E	122	GLY	CA-C	5.83	1.58	1.52
1	E	162	PRO	CA-CB	-5.82	1.44	1.53
1	E	238(A)	LYS	N-CA	-5.79	1.38	1.45
1	E	84	VAL	CA-C	-5.75	1.45	1.52
1	E	174	ALA	CA-C	-5.74	1.44	1.52
1	E	178	SER	CA-C	5.72	1.59	1.52
1	E	30	ASP	N-CA	-5.70	1.39	1.46
1	E	286	GLY	C-N	-5.69	1.25	1.33
1	E	315	ASN	N-CA	5.69	1.53	1.46
1	E	300	ASN	C-O	5.68	1.30	1.23
1	E	261	VAL	C-O	-5.67	1.17	1.24
1	E	241	SER	N-CA	5.67	1.53	1.46
1	E	10	LEU	CA-C	5.66	1.60	1.52
1	E	18	VAL	C-O	-5.66	1.18	1.24
1	E	121	LEU	C-N	5.64	1.39	1.33
1	E	166	ASN	N-CA	5.64	1.53	1.45
1	E	273	ILE	CA-CB	-5.62	1.47	1.54
1	E	234	GLN	CD-OE1	5.61	1.34	1.23
1	E	115	SER	C-N	-5.60	1.25	1.33
1	E	1	SER	CA-C	5.57	1.59	1.52
1	E	127	THR	CA-C	5.55	1.60	1.52
1	E	287	ILE	CA-CB	-5.53	1.47	1.53
1	E	153	ALA	CA-CB	-5.50	1.45	1.53
1	E	191	GLU	C-N	-5.50	1.26	1.33
1	E	190	TRP	CA-CB	-5.48	1.45	1.52
1	E	306	ALA	CA-C	-5.46	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	SER	CA-C	-5.45	1.45	1.52
1	E	147	ASP	CA-C	5.44	1.60	1.52
1	E	141	ASN	CG-OD1	5.42	1.33	1.23
1	E	261	VAL	CA-CB	-5.41	1.46	1.53
1	E	50	VAL	CA-CB	-5.38	1.47	1.53
1	E	298	GLY	N-CA	5.35	1.52	1.45
1	E	175	TYR	C-N	-5.34	1.25	1.33
1	E	258	THR	CA-CB	5.34	1.62	1.53
1	E	80(A)	SER	N-CA	-5.32	1.39	1.46
1	E	99	GLN	CA-CB	5.31	1.61	1.53
1	E	150	VAL	C-N	-5.29	1.26	1.33
1	E	319	THR	CB-OG1	5.25	1.52	1.43
1	E	135	GLN	CD-OE1	5.24	1.33	1.23
1	E	99	GLN	CD-OE1	5.22	1.33	1.23
1	E	308	LYS	C-N	-5.22	1.25	1.33
1	E	138	PHE	N-CA	5.21	1.52	1.46
1	E	155	LEU	N-CA	5.14	1.52	1.46
1	E	178	SER	N-CA	5.13	1.52	1.45
1	E	263	SER	CA-C	-5.13	1.45	1.52
1	E	159	ALA	N-CA	5.13	1.53	1.46
1	E	304	ASP	CA-C	-5.13	1.45	1.52
1	E	119	GLY	C-N	-5.13	1.25	1.33
1	E	212	GLY	C-O	-5.01	1.18	1.23
1	E	25	GLN	CD-OE1	5.01	1.33	1.23

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ASP	CA-C-O	16.27	127.38	117.94
1	E	75	TYR	CA-C-N	13.25	134.87	120.03
1	E	75	TYR	C-N-CA	13.25	134.87	120.03
1	E	51	ASP	CA-CB-CG	12.41	125.01	112.60
1	E	151	PHE	O-C-N	-11.67	109.75	123.41
1	E	236	SER	O-C-N	11.23	134.02	122.12
1	E	248	PHE	CA-CB-CG	-11.17	102.63	113.80
1	E	151	PHE	CA-C-O	10.99	134.06	120.54
1	E	266	ILE	O-C-N	10.45	134.28	123.20
1	E	35	SER	CA-C-O	-10.08	110.67	121.45
1	E	319(A)	PRO	O-C-N	-10.05	110.55	123.01
1	E	225	ALA	O-C-N	-9.96	111.56	122.12
1	E	56	TYR	O-C-N	9.68	134.26	123.22
1	E	38	LEU	CA-C-N	-9.37	107.04	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	38	LEU	C-N-CA	-9.37	107.04	122.21
1	E	51	ASP	CB-CA-C	-9.21	103.81	117.07
1	E	272	TYR	N-CA-C	-9.13	101.40	112.54
1	E	319(A)	PRO	CA-C-O	8.97	131.97	121.56
1	E	43	SER	O-C-N	-8.91	110.74	122.33
1	E	278	ILE	CB-CA-C	8.73	123.47	112.04
1	E	174	ALA	N-CA-C	8.69	123.88	113.28
1	E	187	GLN	OE1-CD-NE2	-8.53	114.07	122.60
1	E	149	PRO	CA-C-N	-8.50	111.53	123.17
1	E	149	PRO	C-N-CA	-8.50	111.53	123.17
1	E	86	THR	CA-C-O	-8.42	111.79	120.71
1	E	121	LEU	O-C-N	-8.39	112.04	123.12
1	E	28	ASN	CA-CB-CG	-8.34	104.26	112.60
1	E	280	THR	O-C-N	-8.34	113.05	123.06
1	E	236	SER	CA-C-O	-8.33	111.63	120.63
1	E	91	VAL	CA-CB-CG2	8.11	124.19	110.40
1	E	312	VAL	CA-CB-CG2	8.07	124.11	110.40
1	E	213	ILE	CA-C-O	-8.05	111.25	120.67
1	E	87	ASP	CA-CB-CG	-8.05	104.55	112.60
1	E	51	ASP	CA-C-N	-8.04	105.66	121.41
1	E	51	ASP	C-N-CA	-8.04	105.66	121.41
1	E	275	PHE	CA-CB-CG	-7.98	105.82	113.80
1	E	89	VAL	CA-CB-CG2	7.97	123.95	110.40
1	E	150	VAL	CA-CB-CG1	7.85	123.74	110.40
1	E	266	ILE	CA-C-O	-7.75	112.33	120.39
1	E	60	LYS	CA-C-N	-7.63	112.47	123.00
1	E	60	LYS	C-N-CA	-7.63	112.47	123.00
1	E	56	TYR	CA-C-O	-7.61	111.95	120.54
1	E	151	PHE	CA-CB-CG	7.59	121.39	113.80
1	E	141	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	E	250	CYS	CA-C-N	7.45	133.16	120.72
1	E	250	CYS	C-N-CA	7.45	133.16	120.72
1	E	243	VAL	CA-CB-CG2	7.39	122.97	110.40
1	E	238(A)	LYS	N-CA-C	7.36	120.26	109.07
1	E	31	PHE	CA-CB-CG	-7.33	106.47	113.80
1	E	31	PHE	CA-C-N	7.30	133.95	123.14
1	E	31	PHE	C-N-CA	7.30	133.95	123.14
1	E	263	SER	CA-C-O	7.29	128.44	119.11
1	E	314	PHE	CA-CB-CG	-7.21	106.59	113.80
1	E	313	VAL	CA-CB-CG2	7.19	122.62	110.40
1	E	197	TYR	CA-C-N	7.08	134.54	122.37
1	E	197	TYR	C-N-CA	7.08	134.54	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	300	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	E	185	THR	CA-C-N	7.01	129.99	120.38
1	E	185	THR	C-N-CA	7.01	129.99	120.38
1	E	9	SER	CA-C-N	7.00	133.51	122.60
1	E	9	SER	C-N-CA	7.00	133.51	122.60
1	E	213	ILE	O-C-N	6.95	130.69	123.18
1	E	82	GLY	CA-C-O	-6.94	116.12	120.91
1	E	122	GLY	O-C-N	6.87	130.22	123.35
1	E	211	ASP	CA-CB-CG	-6.87	105.73	112.60
1	E	14	TYR	O-C-N	-6.87	114.27	123.19
1	E	107	VAL	O-C-N	-6.86	115.83	123.03
1	E	273	ILE	CA-CB-CG2	6.83	122.12	110.50
1	E	103	SER	O-C-N	-6.80	115.31	123.13
1	E	259	PHE	CA-C-N	-6.79	114.25	121.45
1	E	259	PHE	C-N-CA	-6.79	114.25	121.45
1	E	107	VAL	CA-CB-CG2	6.71	121.81	110.40
1	E	167	PHE	CA-CB-CG	-6.71	107.09	113.80
1	E	23	PRO	CA-C-N	6.67	130.23	120.82
1	E	23	PRO	C-N-CA	6.67	130.23	120.82
1	E	90	SER	CA-C-N	6.67	131.71	123.17
1	E	90	SER	C-N-CA	6.67	131.71	123.17
1	E	85	TYR	CA-C-O	-6.66	113.64	121.44
1	E	142	ALA	N-CA-C	-6.64	104.65	112.89
1	E	39	TRP	CA-C-N	-6.61	113.31	122.69
1	E	39	TRP	C-N-CA	-6.61	113.31	122.69
1	E	253	THR	N-CA-C	-6.59	97.98	108.73
1	E	121	LEU	CA-C-O	6.59	127.32	120.40
1	E	314	PHE	CA-C-O	6.58	127.76	120.92
1	E	310	ALA	CA-C-N	6.54	131.47	122.77
1	E	310	ALA	C-N-CA	6.54	131.47	122.77
1	E	232	TRP	CZ3-CH2-CZ2	-6.52	113.02	121.50
1	E	288	GLN	CA-C-O	-6.50	113.85	121.46
1	E	278	ILE	CA-CB-CG1	6.49	121.44	110.40
1	E	75	TYR	O-C-N	-6.47	115.34	122.84
1	E	35	SER	O-C-N	6.43	130.49	123.10
1	E	132	SER	C-N-CD	-6.42	106.47	120.60
1	E	125	PHE	CA-CB-CG	-6.42	107.38	113.80
1	E	13	ALA	CA-C-O	-6.39	114.07	121.10
1	E	3	THR	CA-C-N	-6.39	112.78	122.81
1	E	3	THR	C-N-CA	-6.39	112.78	122.81
1	E	49	GLU	N-CA-CB	6.39	120.05	110.53
1	E	124	ALA	CA-C-O	-6.37	113.54	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	121	LEU	CA-C-N	-6.33	115.44	121.57
1	E	121	LEU	C-N-CA	-6.33	115.44	121.57
1	E	237	GLY	CA-C-O	6.33	128.07	119.28
1	E	28	ASN	O-C-N	-6.31	115.54	123.05
1	E	301	ILE	N-CA-C	6.31	117.84	107.24
1	E	305	VAL	CA-CB-CG1	6.31	121.12	110.40
1	E	164	THR	O-C-N	6.30	130.58	123.27
1	E	232	TRP	CE3-CZ3-CH2	6.29	129.28	121.10
1	E	308	LYS	CB-CG-CD	-6.26	96.89	111.30
1	E	299	ILE	CA-C-O	-6.24	114.22	120.90
1	E	282(B)	SER	CA-C-O	-6.24	113.88	120.80
1	E	116	THR	CA-C-N	6.23	131.48	123.13
1	E	116	THR	C-N-CA	6.23	131.48	123.13
1	E	187	GLN	CG-CD-NE2	6.20	125.70	116.40
1	E	306	ALA	CA-C-N	6.19	128.57	120.28
1	E	306	ALA	C-N-CA	6.19	128.57	120.28
1	E	193	THR	N-CA-C	6.17	118.82	108.02
1	E	238(A)	LYS	CA-CB-CG	-6.16	101.78	114.10
1	E	297	ILE	N-CA-C	-6.16	104.28	111.00
1	E	34	GLY	CA-C-N	6.16	131.97	121.87
1	E	34	GLY	C-N-CA	6.16	131.97	121.87
1	E	303	GLY	CA-C-N	6.16	128.81	120.38
1	E	303	GLY	C-N-CA	6.16	128.81	120.38
1	E	324	ALA	N-CA-CB	6.12	122.08	111.00
1	E	282(B)	SER	O-C-N	6.12	130.35	123.19
1	E	297	ILE	O-C-N	-6.10	113.79	121.84
1	E	231	TYR	CA-CB-CG	-6.09	102.94	113.90
1	E	71	TRP	CA-C-N	6.07	131.41	121.58
1	E	71	TRP	C-N-CA	6.07	131.41	121.58
1	E	80(A)	SER	O-C-N	-6.06	116.93	123.42
1	E	279	SER	CA-C-O	-6.03	114.06	121.06
1	E	98	GLY	O-C-N	-6.03	114.99	122.34
1	E	14	TYR	CA-C-O	6.01	127.90	121.11
1	E	43	SER	CA-C-N	5.97	133.17	122.06
1	E	43	SER	C-N-CA	5.97	133.17	122.06
1	E	232	TRP	CB-CG-CD1	-5.97	117.95	126.90
1	E	63	THR	CA-C-O	5.96	126.50	119.28
1	E	218	THR	N-CA-CB	5.95	119.91	110.57
1	E	321	LEU	CA-C-N	5.94	128.56	122.80
1	E	321	LEU	C-N-CA	5.94	128.56	122.80
1	E	122	GLY	CA-C-O	-5.93	115.96	121.18
1	E	184	VAL	CA-CB-CG2	5.92	120.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	79	SER	CA-C-N	-5.92	110.78	121.62
1	E	79	SER	C-N-CA	-5.92	110.78	121.62
1	E	244	GLY	O-C-N	-5.92	115.90	122.47
1	E	156	GLY	CA-C-N	-5.90	115.17	122.84
1	E	156	GLY	C-N-CA	-5.90	115.17	122.84
1	E	113	GLU	CA-C-N	-5.90	114.04	122.77
1	E	113	GLU	C-N-CA	-5.90	114.04	122.77
1	E	10	LEU	CB-CA-C	-5.89	100.77	110.72
1	E	140	ASP	CA-CB-CG	-5.87	106.73	112.60
1	E	236	SER	N-CA-CB	5.87	118.86	110.06
1	E	294	SER	CA-C-N	5.87	129.62	120.82
1	E	294	SER	C-N-CA	5.87	129.62	120.82
1	E	221	LEU	O-C-N	-5.86	115.67	122.87
1	E	2	ALA	O-C-N	-5.85	116.14	123.27
1	E	133	PRO	CA-C-N	-5.84	114.76	122.99
1	E	133	PRO	C-N-CA	-5.84	114.76	122.99
1	E	25	GLN	OE1-CD-NE2	-5.83	116.77	122.60
1	E	215	ASP	N-CA-CB	-5.83	100.86	110.95
1	E	48	SER	CA-C-N	5.81	132.31	122.26
1	E	48	SER	C-N-CA	5.81	132.31	122.26
1	E	135	GLN	N-CA-C	-5.80	100.25	109.59
1	E	261	VAL	N-CA-CB	5.80	119.25	112.35
1	E	253	THR	O-C-N	-5.77	116.64	123.22
1	E	315	ASN	CB-CG-ND2	5.76	125.04	116.40
1	E	50	VAL	N-CA-C	5.76	116.09	107.51
1	E	215	ASP	CA-CB-CG	-5.74	106.86	112.60
1	E	154	ASP	CA-C-N	-5.73	113.61	122.09
1	E	154	ASP	C-N-CA	-5.73	113.61	122.09
1	E	54	THR	CA-C-N	-5.72	114.22	122.45
1	E	54	THR	C-N-CA	-5.72	114.22	122.45
1	E	108	SER	CA-C-N	5.72	127.94	120.28
1	E	108	SER	C-N-CA	5.72	127.94	120.28
1	E	230	ALA	CA-C-N	5.71	128.18	120.65
1	E	230	ALA	C-N-CA	5.71	128.18	120.65
1	E	307	LEU	N-CA-CB	5.68	118.48	110.12
1	E	258	THR	N-CA-CB	-5.68	101.54	110.69
1	E	34	GLY	CA-C-O	-5.66	111.96	119.10
1	E	203(A)	PHE	N-CA-CB	5.66	119.09	109.87
1	E	43	SER	N-CA-C	-5.65	105.00	112.34
1	E	178	SER	N-CA-C	-5.65	100.83	109.41
1	E	159	ALA	N-CA-CB	-5.64	100.33	110.37
1	E	169	PHE	N-CA-CB	5.64	120.30	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	ALA	N-CA-C	5.63	117.86	111.11
1	E	84	VAL	N-CA-C	5.63	116.84	108.46
1	E	232	TRP	CB-CG-CD2	5.62	134.67	126.80
1	E	10	LEU	CA-C-O	-5.62	112.96	119.59
1	E	50	VAL	CA-CB-CG2	5.59	119.90	110.40
1	E	159	ALA	CA-C-N	-5.59	114.84	120.21
1	E	159	ALA	C-N-CA	-5.59	114.84	120.21
1	E	286	GLY	CA-C-N	5.59	130.71	123.11
1	E	286	GLY	C-N-CA	5.59	130.71	123.11
1	E	235	VAL	CA-C-N	5.57	128.01	120.38
1	E	235	VAL	C-N-CA	5.57	128.01	120.38
1	E	25	GLN	CG-CD-NE2	5.54	124.71	116.40
1	E	33	THR	CA-C-O	5.53	127.76	118.91
1	E	50	VAL	CA-CB-CG1	5.53	119.79	110.40
1	E	111	PHE	CA-C-N	5.53	127.69	120.28
1	E	111	PHE	C-N-CA	5.53	127.69	120.28
1	E	236	SER	N-CA-C	5.51	118.00	111.33
1	E	132	SER	O-C-N	-5.51	116.32	121.72
1	E	31	PHE	O-C-N	-5.50	115.34	122.77
1	E	268	ILE	CB-CA-C	-5.50	104.46	110.78
1	E	314	PHE	CA-C-N	-5.49	115.12	122.42
1	E	314	PHE	C-N-CA	-5.49	115.12	122.42
1	E	190	TRP	N-CA-C	-5.46	100.71	109.39
1	E	255	PRO	O-C-N	-5.45	116.35	123.00
1	E	182	THR	O-C-N	-5.45	116.62	123.27
1	E	246	TYR	CA-C-N	5.43	131.33	122.69
1	E	246	TYR	C-N-CA	5.43	131.33	122.69
1	E	135	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	E	167	PHE	O-C-N	5.41	129.64	123.31
1	E	80	SER	C-N-CA	5.41	135.22	121.70
1	E	315	ASN	N-CA-CB	-5.39	101.63	110.21
1	E	117	ILE	CA-C-O	5.39	126.41	120.48
1	E	84	VAL	CA-CB-CG2	5.39	119.56	110.40
1	E	133	PRO	CA-N-CD	5.38	119.03	111.50
1	E	169	PHE	CA-C-O	-5.38	115.48	121.23
1	E	32	ASP	N-CA-C	5.37	118.20	107.62
1	E	248	PHE	CA-C-O	-5.34	115.42	120.34
1	E	220	LEU	CB-CA-C	-5.33	101.13	112.63
1	E	86	THR	N-CA-C	-5.30	101.06	109.59
1	E	315	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	E	266	ILE	N-CA-C	-5.28	100.04	107.75
1	E	39	TRP	N-CA-C	-5.27	101.28	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	15	ILE	O-C-N	5.26	128.56	123.03
1	E	80(A)	SER	N-CA-CB	5.25	119.70	111.56
1	E	51	ASP	N-CA-C	-5.25	104.47	108.78
1	E	311	PHE	N-CA-C	-5.24	100.19	108.73
1	E	225	ALA	CB-CA-C	-5.24	102.09	110.79
1	E	261	VAL	O-C-N	5.24	127.79	122.71
1	E	138	PHE	CA-C-O	5.24	126.10	120.55
1	E	294	SER	CA-C-O	-5.23	113.44	119.56
1	E	13	ALA	O-C-N	5.22	128.63	123.46
1	E	238(A)	LYS	O-C-N	-5.22	117.30	123.25
1	E	49	GLU	CA-C-N	5.20	129.74	122.93
1	E	49	GLU	C-N-CA	5.20	129.74	122.93
1	E	315	ASN	O-C-N	-5.19	116.70	122.93
1	E	270	GLY	CA-C-O	-5.17	115.73	120.80
1	E	41	PHE	O-C-N	-5.15	116.78	122.86
1	E	325	SER	O-C-N	-5.14	116.79	122.86
1	E	103	SER	CA-C-O	5.12	126.16	120.43
1	E	164	THR	CA-C-O	-5.11	115.14	121.06
1	E	274	ASP	CA-C-N	-5.10	113.51	120.44
1	E	274	ASP	C-N-CA	-5.10	113.51	120.44
1	E	304	ASP	N-CA-C	5.09	117.49	111.33
1	E	248	PHE	N-CA-C	5.09	114.16	108.25
1	E	158	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	E	39	TRP	N-CA-CB	-5.07	102.88	111.69
1	E	147	ASP	N-CA-C	-5.05	105.91	111.71
1	E	233	ALA	CA-C-O	-5.05	113.17	119.38
1	E	30	ASP	CB-CG-OD1	5.04	130.00	118.40
1	E	150	VAL	N-CA-CB	-5.03	104.01	112.06
1	E	203	THR	C-N-CA	5.03	134.28	121.70
1	E	232	TRP	CD2-CE2-CZ2	5.03	127.43	122.40
1	E	237	GLY	CA-C-N	-5.03	114.23	121.42
1	E	237	GLY	C-N-CA	-5.03	114.23	121.42
1	E	144	ALA	CA-C-N	5.02	129.93	121.14
1	E	144	ALA	C-N-CA	5.02	129.93	121.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2389	0	2280	21	1
2	E	10	0	0	0	0
3	E	47	0	57	18	0
4	E	260	0	0	1	3
All	All	2706	0	2337	39	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:333:1Z1:HD12	3:E:333:1Z1:CD11	0.97	1.14
3:E:333:1Z1:CD11	3:E:333:1Z1:HD13	0.97	1.11
3:E:333:1Z1:CD11	3:E:333:1Z1:HD11	0.97	1.08
3:E:333:1Z1:HD25	3:E:333:1Z1:CD21	0.97	1.07
3:E:333:1Z1:CD12	3:E:333:1Z1:HD14	0.97	1.06
3:E:333:1Z1:CE2	3:E:333:1Z1:CG4	2.40	0.94
3:E:333:1Z1:HD14	3:E:333:1Z1:CG4	1.99	0.91
3:E:333:1Z1:HD12	3:E:333:1Z1:CG	2.04	0.88
3:E:333:1Z1:HD11	3:E:333:1Z1:CG	2.04	0.87
3:E:333:1Z1:HD13	3:E:333:1Z1:CG	2.04	0.86
3:E:333:1Z1:CG4	3:E:333:1Z1:CE1	2.47	0.86
3:E:333:1Z1:HD12	3:E:333:1Z1:HD13	1.58	0.85
3:E:333:1Z1:HD14	3:E:333:1Z1:CE1	2.05	0.85
3:E:333:1Z1:HD12	3:E:333:1Z1:HD11	1.58	0.84
3:E:333:1Z1:HD13	3:E:333:1Z1:HD11	1.58	0.83
3:E:333:1Z1:HD25	3:E:333:1Z1:CE2	2.07	0.83
3:E:333:1Z1:HD25	3:E:333:1Z1:CG4	2.08	0.82
1:E:129:ASN:ND2	1:E:135:GLN:H	1.93	0.66
1:E:18:VAL:HG21	1:E:29:LEU:HD12	1.81	0.63
1:E:114:ASP:OD2	1:E:117:ILE:HD12	2.00	0.62
1:E:5:THR:HG22	1:E:162:PRO:HB3	1.85	0.59
1:E:129:ASN:HD21	1:E:131:VAL:HB	1.71	0.55
1:E:198:ALA:HB2	1:E:203(A):PHE:HA	1.92	0.51
1:E:39:TRP:HA	1:E:102:GLU:O	2.11	0.50
1:E:129:ASN:ND2	1:E:131:VAL:H	2.11	0.48
1:E:277:PRO:HA	1:E:283:CYS:HA	1.95	0.48
3:E:333:1Z1:HE2	3:E:333:1Z1:HB3	1.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:SER:HB3	1:E:110:SER:OG	2.15	0.46
1:E:231:TYR:OH	1:E:255:PRO:HD2	2.15	0.46
1:E:60:LYS:HE2	1:E:60:LYS:HA	2.00	0.44
1:E:220:LEU:HD22	1:E:286:GLY:HA2	2.01	0.43
1:E:99:GLN:NE2	1:E:138:PHE:HA	2.35	0.42
1:E:114:ASP:HB2	4:E:548:HOH:O	2.19	0.42
1:E:121:LEU:C	1:E:121:LEU:HD23	2.44	0.42
1:E:152:THR:HG22	1:E:313:VAL:HG22	2.01	0.42
1:E:51:ASP:HB3	1:E:52:GLY:H	1.31	0.42
1:E:28:ASN:HD22	1:E:28:ASN:HA	1.68	0.41
1:E:41:PHE:HB3	1:E:55:ILE:HG22	2.03	0.41
1:E:194:SER:HB3	1:E:207:ILE:HB	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:533:HOH:O	4:E:593:HOH:O[1_655]	0.42	1.78
4:E:554:HOH:O	4:E:569:HOH:O[2_656]	1.71	0.49
1:E:319:THR:OG1	4:E:583:HOH:O[2_555]	1.85	0.35

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	328/330 (99%)	321 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	263/263 (100%)	252 (96%)	11 (4%)	26	19

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	51	ASP
1	E	79	SER
1	E	120	LEU
1	E	150	VAL
1	E	170	ILE
1	E	186	LYS
1	E	204	LYS
1	E	204(A)	SER
1	E	251	SER
1	E	278	ILE
1	E	299	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	28	ASN
1	E	99	GLN
1	E	129	ASN
1	E	135	GLN
1	E	141	ASN
1	E	166	ASN
1	E	300	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	E	327	-	4,4,4	0.24	0	6,6,6	0.16	0
3	1Z1	E	333	-	45,47,47	2.66	10 (22%)	58,62,62	2.94	25 (43%)
2	SO4	E	328	-	4,4,4	0.52	0	6,6,6	1.22	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1Z1	E	333	-	-	13/60/60/60	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	333	1Z1	C2-N3	10.29	1.42	1.32
3	E	333	1Z1	O11-S1	8.80	1.52	1.43
3	E	333	1Z1	C2-NZ	5.95	1.43	1.33
3	E	333	1Z1	O21-S1	-4.92	1.37	1.43
3	E	333	1Z1	C21-N5	3.64	1.52	1.47
3	E	333	1Z1	CA1-N1	3.22	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	333	1Z1	CH-CA1	2.50	1.57	1.53
3	E	333	1Z1	CE1-CD12	2.16	1.42	1.38
3	E	333	1Z1	CD2-CG	2.11	1.62	1.51
3	E	333	1Z1	C11-N5	2.05	1.50	1.47

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	333	1Z1	CM1-N3-C2	-12.74	113.64	124.13
3	E	333	1Z1	CE-NZ-C2	-7.37	112.67	124.67
3	E	333	1Z1	O21-S1-O11	-6.37	108.44	119.80
3	E	333	1Z1	C21-N5-C11	-4.64	105.54	114.75
3	E	333	1Z1	O21-S1-N5	4.14	113.74	107.13
3	E	333	1Z1	CE1-CD12-CG4	3.94	126.16	120.61
3	E	333	1Z1	O21-S1-N4	3.59	117.10	107.63
3	E	333	1Z1	CZ-CE1-CD12	-3.59	115.81	120.24
3	E	333	1Z1	S-C2-N3	-3.54	118.54	123.66
3	E	333	1Z1	CA-N-C	-3.21	115.80	122.69
3	E	333	1Z1	C11-N5-S1	-3.17	107.08	117.71
3	E	333	1Z1	CB2-CA2-N2	3.05	116.94	110.91
3	E	333	1Z1	C21-N5-S1	-2.95	107.83	117.71
3	E	333	1Z1	CA1-N1-C1	-2.88	118.23	123.25
3	E	333	1Z1	CM-C-N	2.88	120.42	115.97
3	E	333	1Z1	CB2-CA2-C1	2.77	116.89	110.11
3	E	333	1Z1	CG3-CD-CE	-2.70	101.08	113.56
3	E	333	1Z1	O11-S1-N5	-2.66	102.88	107.13
3	E	333	1Z1	CG-CB1-CA1	2.45	120.48	115.54
3	E	333	1Z1	CA2-N2-C3	2.45	126.91	121.65
3	E	333	1Z1	CD-CG3-CB2	-2.33	104.85	113.62
3	E	333	1Z1	CZ-CE2-CD21	2.29	123.06	120.24
3	E	333	1Z1	NZ-C2-N3	2.19	120.22	116.14
2	E	328	SO4	O3-S-O1	2.17	120.89	109.56
3	E	333	1Z1	O-C-CM	-2.06	118.52	121.54
3	E	333	1Z1	CB1-CA1-CH	-2.06	109.43	112.55

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	333	1Z1	CA3-N4-S1-N5
3	E	333	1Z1	C21-N5-S1-N4
3	E	333	1Z1	C21-N5-S1-O11

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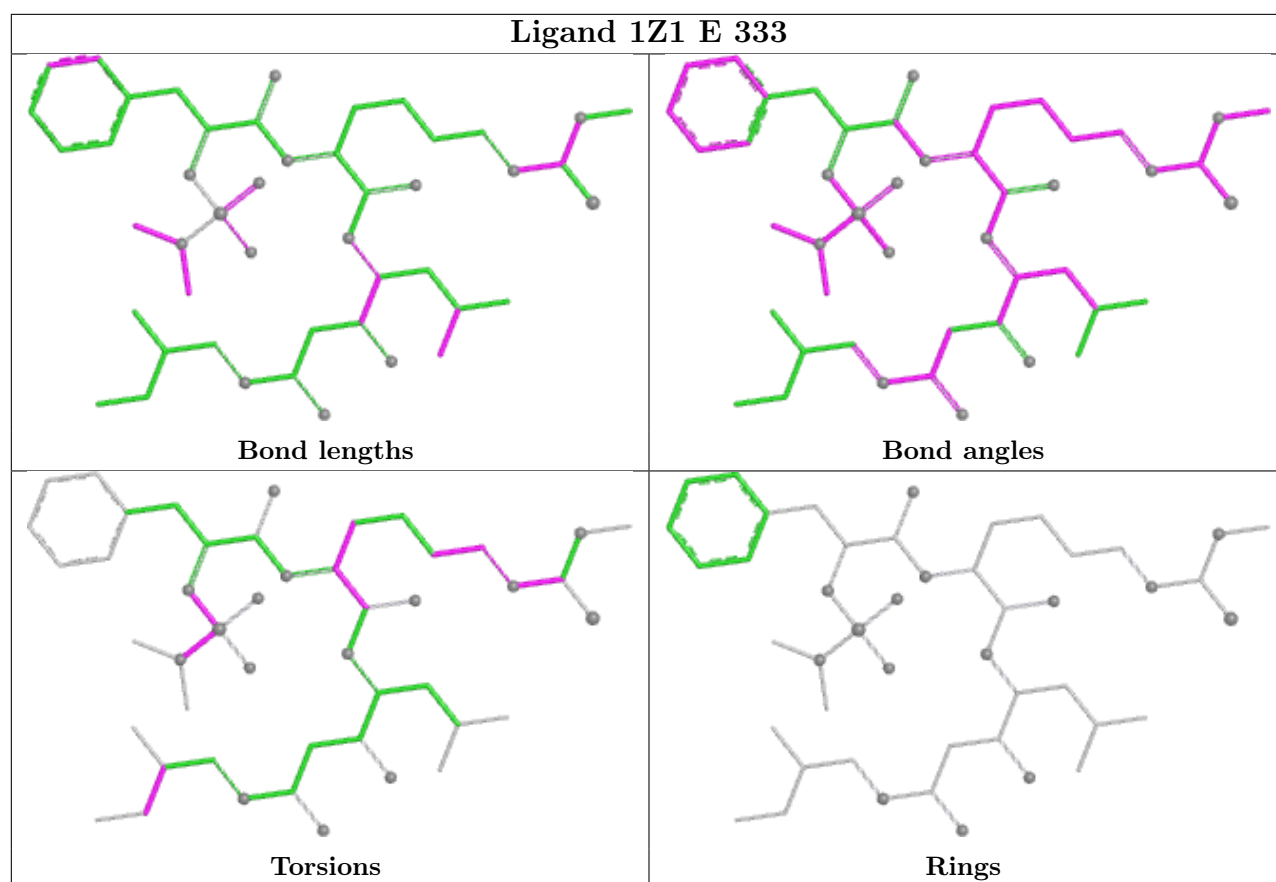
Mol	Chain	Res	Type	Atoms
3	E	333	1Z1	C11-N5-S1-O21
3	E	333	1Z1	N2-CA2-CB2-CG3
3	E	333	1Z1	CG3-CD-CE-NZ
3	E	333	1Z1	C1-CA2-CB2-CG3
3	E	333	1Z1	CG2-CB-CG1-CD1
3	E	333	1Z1	O1-C1-CA2-N2
3	E	333	1Z1	N1-C1-CA2-N2
3	E	333	1Z1	S-C2-NZ-CE
3	E	333	1Z1	N3-C2-NZ-CE
3	E	333	1Z1	CD-CE-NZ-C2

There are no ring outliers.

1 monomer is involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	333	1Z1	18	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.